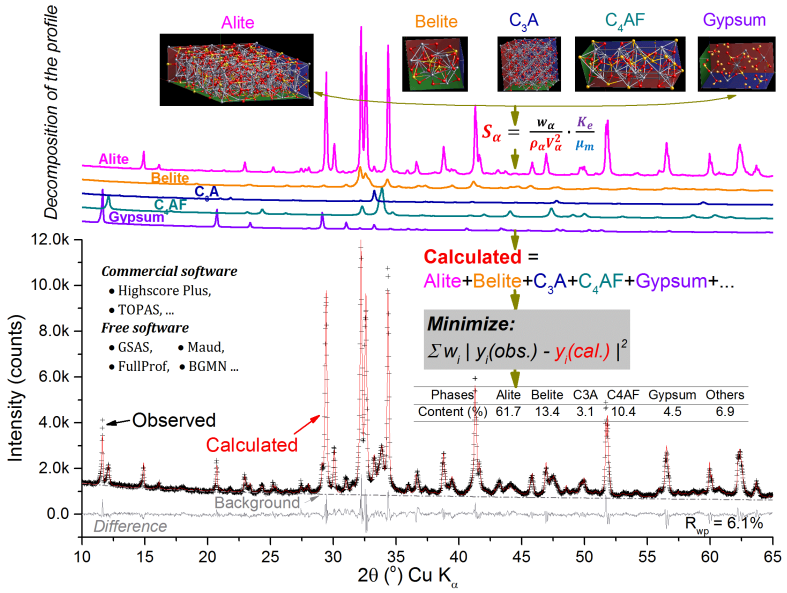
What is the Rietveld analysis

- ***Method for quantification***
- ***Compare experimental pattern to the calculated one. The crystal structure of the phases are used and refined to match the experimental pattern by minimizing the difference between the experimental and calculated patterns.***



*For phase **α** in the mixture [1]:*

$$S_\alpha = \frac{w_\alpha}{\rho_\alpha V_\alpha^2} \cdot \frac{K_e}{\mu_m} \qquad \text{eq. (1)}$$

w_α: weight fraction, S_α: scale factor; ρ_α: density; V_α: unit cell volume; μ_m: mass absorption coefficient; K_e: experimental constant.

Rearrange eq. (1) to get the weight faction:

$$w_\alpha = S_\alpha \cdot \rho_\alpha V_\alpha^2 \cdot \frac{\mu_m}{K_e} \qquad \text{eq. (2)}$$

❖ ***Default Rietveld output**:*

Assume no amorphous present: $\sum w_i = 1$*:*

$$w_\alpha = (S_\alpha \rho_\alpha V_\alpha^2) / \sum S_i \rho_i V_i^2$$

*When **internal standard** w_s added into the sample, then*

$$Amorphous = \left(1 - w_s^{weighed} / w_s^{Rietveld}\right) / \left(1 - w_s^{weighed}\right)$$

❖ ***External standard method** (K or G factor)[2]:*

Get K_e *using standard:* $K_e = {}^{S_s \cdot \rho_s V_s^2 \cdot \mu_m}/_{w_s}$ *; calculate* μ_m *with chemical composition,* w_α *can be obtained from eq. (2), which is the absolute content,*

$$Amorphous = 1 - \sum w_i$$

❖ ***PONKCS method**[3]:*

For amorphous phases with characteristic 'hump', $\rho_\alpha V_\alpha^2$ *unknown but can be calibrated and used for quantification in eq.(2):*

$$\rho_{ponkcs} V_{ponkcs}^2 = (K_e w_{ponkcs}) / (\mu_m S_{ponkcs})$$

Reference :[1] M. A. G. Aranda, et al., Rietveld Quantitative Phase Analysis of OPC Clinkers, Cements and Hydration Products, *Rev. Mineral. Geochem., 2012,* 74(1): 169-209; [2] B. H. O'Connor, M. D. Raven, Application of the Rietveld Refinement Procedure in Assaying Powdered Mixtures. Powder Diffr., 1988, 3(01): 2-6; [3] N.V.Y. Scarlett, I.C. Madsen, Quantification of phases with partial or no known crystal structures. Powder Diffr., 2006. 21(04): p. 278-284.